ASCEM/NRAP Integration Workshop Summary

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Hosting Organizations

ASCEM/NRAP Program Integration Workshop Summary

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1.0 Executive Summary

Computational modeling and simulation are at the core of several new initiatives within the Department of Energy (DOE). These efforts are aimed at providing a science-based predictive modeling approach to further understand risk and other challenging problems facing the DOE with respect to subsurface contaminant transport and carbon capture and storage.

The topics of multiphase flow, chemical reactions, heat and mass transfer in subsurface media are crucial across the spectrum of DOE energy initiatives, including environmental stewardship (e.g., nuclear waste disposal), engineered geothermal systems, environmentally sound and efficient production of fossil fuels (both conventional and unconventional), geological storage of CO_2, and management and production of water resources. Decisions in these areas require advanced predictive capabilities for accurately quantifying the behavior of natural systems including coupled physical processes (e.g., multiphase flow, heat/mass transport, biogeochemical reactions, and geomechanical responses) that occur over multiple length and time scales and for which properties of which are inherently heterogeneous and uncertain. Future challenges require the integration of new computational tools with new observations on the behavior and properties of geomaterials and geosystems. DOE has two new initiatives charged with building this new predictive capability:

- Advanced Simulation Capability for Environmental Management (ASCEM) in the area of science-based risk assessment for environmental stewardship
- National Risk Assessment Partnership (NRAP) in the area of geologic storage of CO_2.

At the request of Assistant Secretaries Inés Triay and Jim Markowsky, a workshop was held to investigate potential synergies between DOE Office of Environmental Management's (DOE-EM) ASCEM initiative and DOE Office of Fossil Energy's (DOE-FE) NRAP to facilitate leveraging and coordination between the two programs.

The ASCEM and NRAP initiatives are both designed to enable science-based risk assessment methodologies through the use of best-in-class computational methods to integrate theory and observation. ASCEM is focusing efforts on the development of a state-of-the-art ***scientific tool and approach*** for understanding and predicting contaminant fate and transport in natural and engineered systems, whereas NRAP is focused on developing a science-based methodology for quantifying potential long-term risk (and liability) associated with geologic storage of CO2.

While the two efforts address distinctly different energy challenges facing the DOE, there is potential for synergy between the efforts. Both programs will focus research and development (R&D) on improving computational models and methodologies and quantifying uncertainties to uncover the most important knowledge gaps associated with the long-term fate and transport of fluids and chemical species in the natural environment.

Given these similarities, the workshop participants (representing key technical and programmatic leads from each initiative) discussed the commonalities and differences that emerge when these high-level goals are applied in two distinct application areas: groundwater and soils remediation, and long-term geologic storage of CO_2. Through assessing commonalities and differences, the workshop sought to identify the most efficient means of ensuring integration and coordination across these two important national programs.

Both ASCEM and NRAP are at the early stages of ambitious 5-year research plans. This report outlines the main areas where collaboration is possible between the two programs and makes some recommendations for future action. The workshop was organized around three breakout groups:

1) Computational Platform: A set of computational tools incorporated into a consistent user interface that permit a modeling approach that is flexible, maintains quality and data integrity, and increases user efficiency.
2) V&V / Model Confirmation
3) Multi-Physics Simulator and HPC Framework: A flexible and extensible high performance computational engine that will used to simulate the coupled processes and flow scenarios in the subsurface.

Synergies and collaborations between the two programs were assessed in these technical areas during the workshop.

The workshop highlighted that the two programs have similar goals, but are pursuing different strategies along similar timelines. The ASCEM team is developing a next-generation simulation capability whereas the NRAP team is building on existing best-in-class simulation capabilities and focusing efforts on improving the science base for key processes. NRAP is looking to produce a quantification methodology within the next 3 years, whereas ASCEM is not scheduled to be deployed until 2015. These projects do, however, share significant technical requirements. One likely scenario for significant benefit for these programs is for ASCEM to develop a next-generation simulation platform that can be adapted readily to deploy an NRAP methodology. This approach would allow for a close working relationship to be formed between the two programs as development on the ASCEM simulation capability proceeds.

At the conclusion of this workshop breakout leads and workshop organizers recorded several recommendations formulated from their groups. A common theme discussed at the workshop was the establishment of regular, joint technical exchanges between the programs. The first three recommendations deal specifically with expanding the interactions between the two programs at all levels. The final recommendation deals with establishing an approach for developing tools within the ASCEM program that would benefit the NRAP program in the long-term.

Recommendation 1

Establish a regular dialogue at all levels, from DOE management (DOE-EM/ASCEM, DOE-FE/NRAP, and DOE-Office of Science [SC]) down to the project technical teams. These exchanges could involve both high-level issues as well as more detailed discussions on scheduling of specific deliverables in order to maximize the chances of success for both programs.

Recommendation 2
Hold annual technical exchanges, beginning in the second quarter of FY11, focused on specific areas, including:

- Methodologies for providing community access to and sharing of data, models, and results to facilitate knowledge management
- Approaches for efficient management and integration of data
- Deployment of novel visualization toolsets developed by ASCEM.

In addition, the programs should develop a means to share best practices on the technical issues surrounding the chemical behavior and stability of cement.

Recommendation 3
Establish regular technical exchanges at the working group level to share best practices in Uncertainty Quantification and Verification and Validation. These technical exchanges would involve the ASCEM Site Application effort and relevant NRAP field investigations. The exchange would center on common technical issues surrounding the implementation of the model-driven uncertainty reduction method.

Recommendation 4
Explore a staged approach for extending ASCEM's multi-physics simulator to accommodate NRAP's future requirements. One possible approach would begin with ASCEM's multi-phase capabilities to allow for reservoir modeling, followed by non-isothermal processes, and leading to geo-mechanical coupling. The technical exchanges could be used to communicate NRAP process modeling needs to the ASCEM leadership team for incorporation into the long-term ASCEM high-performance computing (HPC) simulator development. In addition, these exchanges would help define a suite of NRAP-related simulation test cases that could be added to ASCEM's list of benchmarking problems on the HPC simulator.

Recommendation 5
Based on the workshop's success, it was recommended that similar focused "bilateral" workshops be conducted between ASCEM and other programs conducting subsurface science research. This would maximize opportunities to fully educate other DOE Offices on ASCEM's capabilities to address critical DOE missions (e.g., repository science through a combined Office of Environmental Management and Office of Nuclear Energy (EM-NE) workshop, and surface water/groundwater hydrology through an Office of Environmental Management and Office of Science (EM-SC) workshop).

2.0 Background

At the request of Assistant Secretaries Ines Triay and Jim Markowsky, a workshop (See Appendix A: Workshop Agenda, and Appendix B: Workshop Charter) was held to investigate potential synergies between DOE-EM's ASCEM and DOE-FE's NRAP initiatives in order to facilitate leveraging and coordination between programs (including the development of a strategy for potential collaborations and complementary actions). The ASCEM and NRAP initiatives are DOE-funded efforts designed to enable science-based risk assessment methodologies using best-in-class computational methods to integrate theory and observations (laboratory and field-based). Both of these programs will focus R&D efforts on improving computational models/methodologies and quantifying uncertainties to uncover the most important knowledge gaps associated with the long-term fate and transport of fluids and chemical species in the natural environment.

Even though the ASCEM and NRAP initiatives have very similar missions—to enable science-based risk assessment methodologies using best-in-class computational methods to integrate theory, experiments, and observations—they are taking different paths to accomplish these goals in the near-term. These differences result from respective program needs and unique aspects associated with each initiative's specific application areas. Nevertheless, the paths are complementary and are amenable to coordination and integration beneficial to both efforts. The workshop participants (representing key technical and programmatic leads from each initiative) examined the commonalities and differences that emerge when these high-level goals are applied in two distinct application areas: groundwater and soils remediation, and long-term geologic storage of CO_2. The overarching goal of the workshop was to ensure integration and coordination across these two important national programs.

The workshop consisted of overview presentations from both the ASCEM and NRAP teams, followed by more detailed topical areas discussed within smaller breakout sessions (See Appendix C: Workshop Breakout Groups). The topical areas include Computational Platform, V&V / Model Confirmation, and Multi-Physics Simulator and HPC Framework,. For each topical area, participants in the ASCEM and NRAP programs summarized the initiatives' current goals and approaches, compared and contrasted those approaches, and discussed potential avenues to ensure strong coordination and leveraging between the initiatives in order to maximize efficiencies (See Appendix D: Summary Breakout Group Reports).

The ASCEM program is developing a new state-of–the-art HPC computational engine and computational platform with innovative UQ, risk, visualization and data management computing capabilities, whereas NRAP is building on existing best-in-class computational tools and capabilities to meet its near-term program needs, while focusing efforts on improved predictive descriptions for key processes. Both approaches focus R&D efforts on quantifying uncertainties and uncovering the most important knowledge gaps. The use of higher fidelity, science-based models will build confidence in the risk assessment for engineered-natural systems as long as the models themselves are developed through a robust, iterative process to confirm the model's validity for its intended use. In both programs, systems-level models composed of submodels of individual components are required to link source terms, engineered and natural components, and receptors. The computational platform under ASCEM development is flexible, future-ready, and functional on computers from the desktop to the HPC scale, and has the potential for future use in the NRAP program. Finally, for reasons of cost, efficiency, reliability, and credibility, each program has adopted a "common architecture at many sites" paradigm, which promotes standardization of software, methods, and/or approaches through development of a system that can be applied to multiple sites.

Both the ASCEM and NRAP programs are in the early stages of ambitious 5-year research plans, and these aggressive schedules are illustrated in Figures 2.1 and 2.2. A schematic of the high level ASCEM development schedule is illustrated in Figure 2.1. A central goal of ASCEM is to have a fully qualified risk/performance assessment code ready for deployment within EM in 2015. To accomplish this goal and assure a high level of community buy-in of ASCEM's HPC and computational platform capabilities, the ASCEM code will go through a community usage tenure before the code is qualified for regulatory use.

An NRAP central goal is development of a defensible, science-base methodology for quantifying risk profiles and potential long-term liabilities at storage sites within 3-5 years (Figure 2.2), along with an integrated (risk-based) monitoring and mitigation strategy ready to enable commercial deployment of carbon capture and storage by 2016. To accomplish these goals and assure defensibility of the methodology as applied to real systems, NRAP has an extensive effort focused on critical field- and lab-based observations to confirm the predictive methodology in the context of how accurately it captures the preformance of storage sites and their sub-systems.

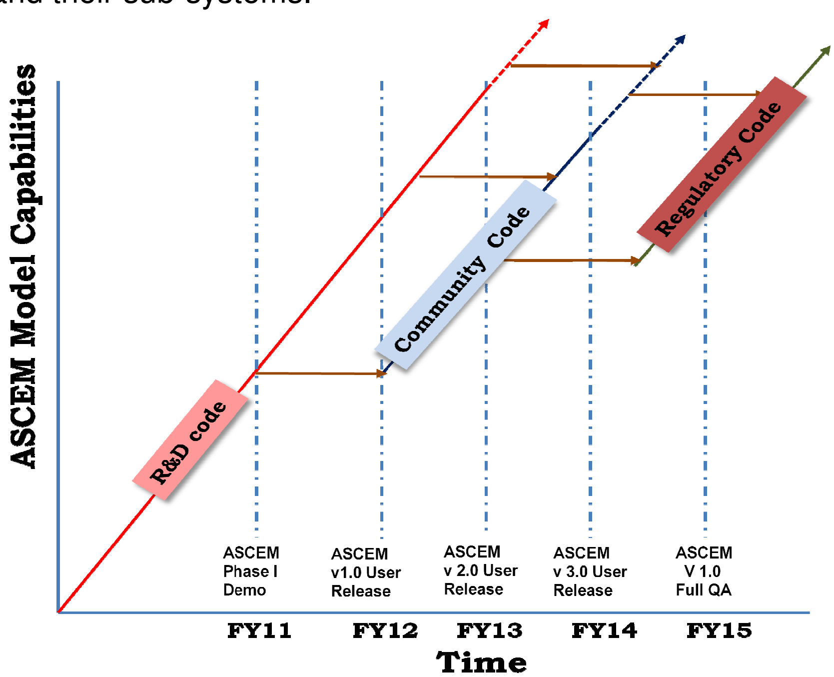

Figure 2.1: High level schematic of ASCEM program schedule illustrating the phased development of the new state-of–the-art HPC computational engine and computational platform with innovative UQ, risk, visualization and data management computing capabilities.

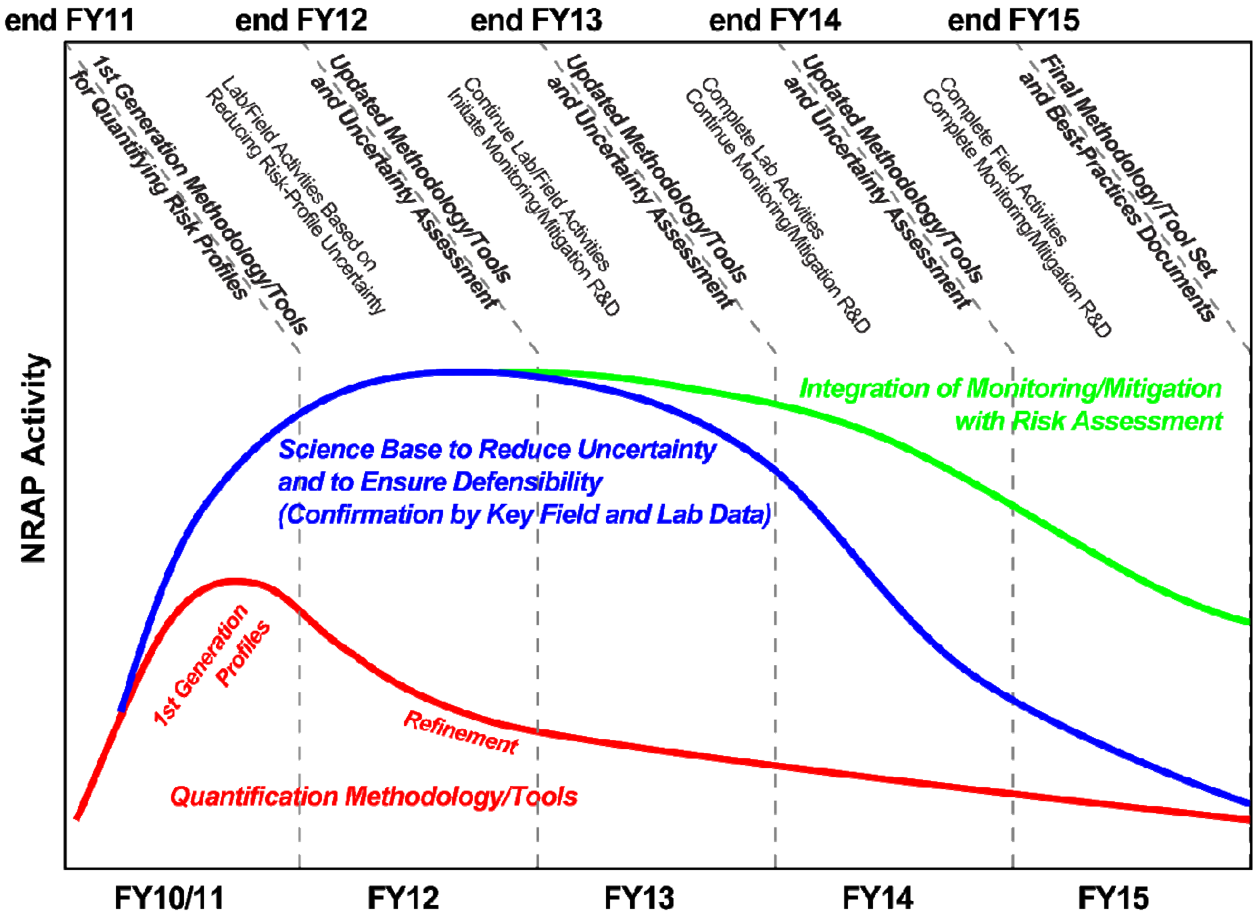

Figure 2.2: High level schematic of NRAP program development schedule illustrating the phased development of the program

3.0 Advanced Simulation Capability for EM - Overview

ASCEM is developing state-of-the-art computational and scientific tools and approaches for integrating data and scientific understanding to enable prediction of contaminant fate and transport in natural and engineered systems. The initiative supports the reduction of uncertainties and risks associated with DOE-EM's environmental cleanup and closure programs by better understanding and quantifying the subsurface flow and contaminant transport behavior in complex geological systems. An additional aspect addresses the long-term performance of engineered components, including cementitious materials in nuclear waste disposal facilities.

The ASCEM modeling initiative will develop an open-source, HPC modeling system for multiphase, multicomponent, multiscale subsurface flow and contaminant transport, and cementitious barrier and source-term degradation. The modeling tools will incorporate capabilities for predicting releases from various waste forms, identifying exposure pathways and performing dose calculations, and conducting systematic uncertainty quantification. ASCEM will demonstrate the modeling tools on selected sites and apply them in support of the next generation of performance assessments of nuclear waste disposal and decommissioning facilities across the EM complex.

A major ASCEM goal is to provide a community code for DOE-EM and the greater scientific and engineering communities. To that end, the ASCEM HPC modeling tools will be developed using an open source model, with involvement from the DOE-SC community. This approach allows ASCEM to leverage the considerable scientific investment that has already been made both within and outside of DOE-EM in the areas of subsurface geosciences, modeling and simulation, and environmental remediation. Through integration of these efforts, ASCEM will facilitate development of more accurate site models, allow for predictive simulation of proposed remediation methods, and play a significant role in preventing the implementation of overly conservative and unnecessarily expensive remediation strategies. Wherever appropriate, ASCEM will use and build upon results and models developed through its associated DOE initiatives.

Within DOE-SC, DOE-NE, and DOE-FE, there are many efforts in the development of advanced HPC capabilities, as well as scientific investigations of groundwater flow and transport, source term degradation and release, and mechanical degradation of structures and barriers. By leveraging these investments, ASCEM will develop a toolset for use not only within DOE-EM, but one also available to the greater DOE community in the areas of geologic carbon sequestration and high-level waste repository performance. ASCEM has already established ties with each of these DOE Offices, and will strengthen them through close interactions during the development cycle and during investigations of new research areas.

The ASCEM project is organized into three technical thrust areas: the Multi-Process High Performance Computing Simulator, which provides the computational engine; the Platform and Integrated Toolsets, which provide the user interfaces; and Site Applications (see Figure 3.1). Detailed descriptions of the three thrust areas are contained in the FY2010 ASCEM Implementation Plan.

3.1 Site Applications Thrust

The Site Applications thrust area provides the main link between ASCEM and the EM community's modeling and regulatory needs; it is vital to ensuring that ASCEM HPC modeling capabilities are widely accepted across the EM Complex. Because engaging the user community will be particularly important in the early stages of the ASCEM development, the Site Applications thrust area incorporates a "user interface" task focused on establishing contact with end users, soliciting their input about ASCEM development plans, and conveying the feedback to members of the HPC and Platform Thrust areas responsible for the tool and code development.

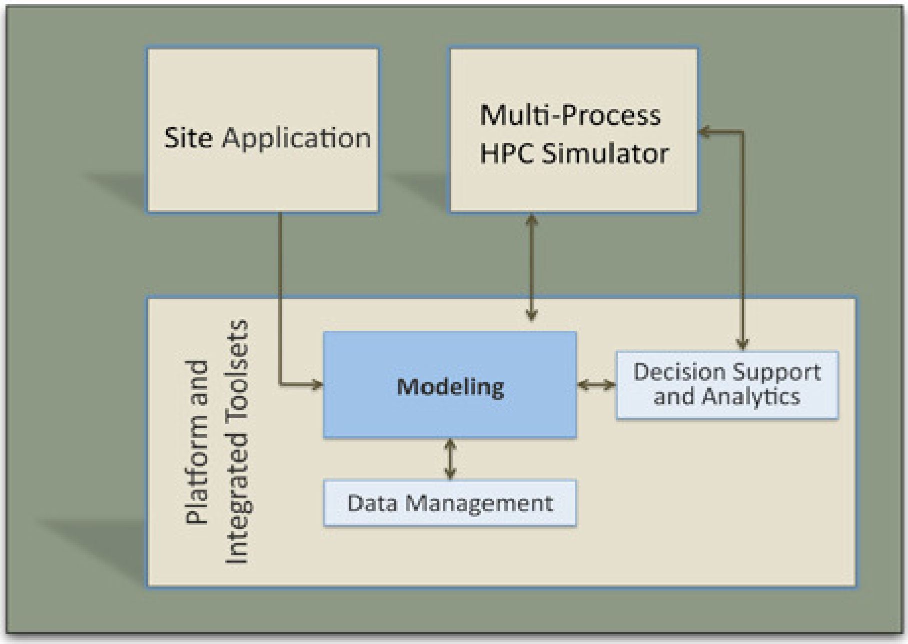

Figure 3.1: The three technical thrust areas of ASCEM: Multi-Process HPC Simulator, Platform and Integrated Toolset, and Site Applications.

3.2 Platform and Integrated Toolsets Thrust

The Platform and Integrated Toolset thrust will provide a standardized user interface enabling end users to create inputs, analyze outputs, and manage data associated with running simulations, and conduct performance and risk assessments. Under this thrust area, ASCEM will use a modular (or "interoperable") approach to code development, facilitating iterative and graded modeling systems that allow end-user customization for specific applications without the need for specialized computational or code development expertise. This will be accomplished by developing programming "interfaces" for each module (where an interface defines access to a module while hiding the details of its implementation). By using a common base platform available to all, this interoperable approach will support cooperation among numerous modeling groups with different methodologies and applications. This methodology has been quite successful in the past and is broadly used in similar advanced software engineering approaches, for example, within the Scientific Discovery Through Advanced Computing (SciDAC) program and the DOE National Nuclear Security Administration Accelerated Strategic Computing (ASC) program. This modular approach will also be used to develop new, more realistic and complete process models that are imperative for successfully implementing performance and risk assessment approaches.

3.3 Multi-Process HPC Simulator Thrust

The third thrust area, the Multi-Process HPC Simulator, will provide the core simulation capabilities necessary for modeling EM sites. The HPC Simulator will provide a flexible and extensible computational engine to simulate the coupled processes and flow scenarios described by the conceptual models developed using the ASCEM Platform. The graded and iterative approach to assessments naturally generates a suite of conceptual models that span a range of process complexity, potentially coupling hydrological, biogeochemical, geomechanical, and thermal processes. To enable this approach, ASCEM will take advantage of emerging petascale computers that handle hundreds of thousands of simultaneous process streams of information. Their use will facilitate improved uncertainty quantification and, when necessary, the use of more complex models in lieu of simplifying assumptions. These HPC-capable tools will be available on platforms from clusters to desktop computers. While there is a clear recognition that many problems will not require the highest end computing capabilities, computer architectures on today's supercomputers will be commonplace on desktop computers in the near future (5-7 years). By developing the ASCEM modeling tools for HPC platforms, this community code will be well positioned to run on a range of platforms, including future desktops.

Finally, the ASCEM modeling capability will be made available to EM site users through training and technology transfer. It will also be made available to the greater scientific community for use in subsurface and risk analysis research and for creating additional modules incorporating scientific advances and new research areas.

4.0 National Risk Assessment Program Overview

NRAP is developing a defensible, science-based methodology for quantifying potential risk associated with long-term CO_2 storage. To achieve this, NRAP is adapting and evolving state-of-the-art scientific tools and approaches for predicting the behavior of engineered natural systems over a variety of length and time scales. NRAP augments DOE-FE's Carbon Sequestration Program by developing risk assessment best practices to evaluate potential long-term liability for a storage site, and to optimize the site characterization, monitoring, and mitigation strategies necessary (pre-operation, syn-operation, and post closure) to reduce both uncertainties and risk. Risk assessments stem from predicting the behavior of the storage-site system in response to the introduction of CO_2, which includes predicting the subsurface fate and impact of the CO_2 and other displaced fluids resulting from coupled flow, reaction, and geomechanical response.

NRAP involves both computational modeling and development of the critical science base necessary to provide the quantitative descriptions of the engineered natural systems at storage sites. Consequently, NRAP will integrate laboratory and field data, both in the development of quantitative descriptions and in the validation of various components of the methodology. The tools and methodologies used to predict multiphase/multiscale flow and, hence, site performance is anticipated to be open-source.

NRAP is not presently focused on development of a HPC modeling platform for three primary reasons. First, many reservoir tools and simulators (mostly non-HPC) are actively being adapted by numerous groups for application to CO_2 in a storage reservoir; the reservoir simulation component of the site-performance assessment must be able to interface with these tools. Second, a first generation methodology for quantifying long-term risk is needed on a short timeline to meet Presidential goals for enabling wide-spread commercial deployment; so, NRAP is emphasizing development of methodologies that can be implemented on any platform (from the current platform(s) under development in NRAP to any future platforms such as the one ASCEM is developing). Finally, much of the uncertainty related to prediction of storage-site performance stems from data limitations (e.g., related to heterogeneous site properties and characteristics), so NRAP is emphasizing the evaluation of these uncertainties and key field/lab studies to reduce the uncertainties.

NRAP is developing a methodology based on an integrated assessment model (IAM), whereby the overall storage site is described by a number of linked subsystems (see Figure 4.1). Organizationally, NRAP is structured around technical working groups that map to key aspects of the IAM as well as system modeling and monitoring (which integrate across the other technical working groups). These working groups define the key technical needs (and, hence, annual research path) for developing a quantitative methodology.

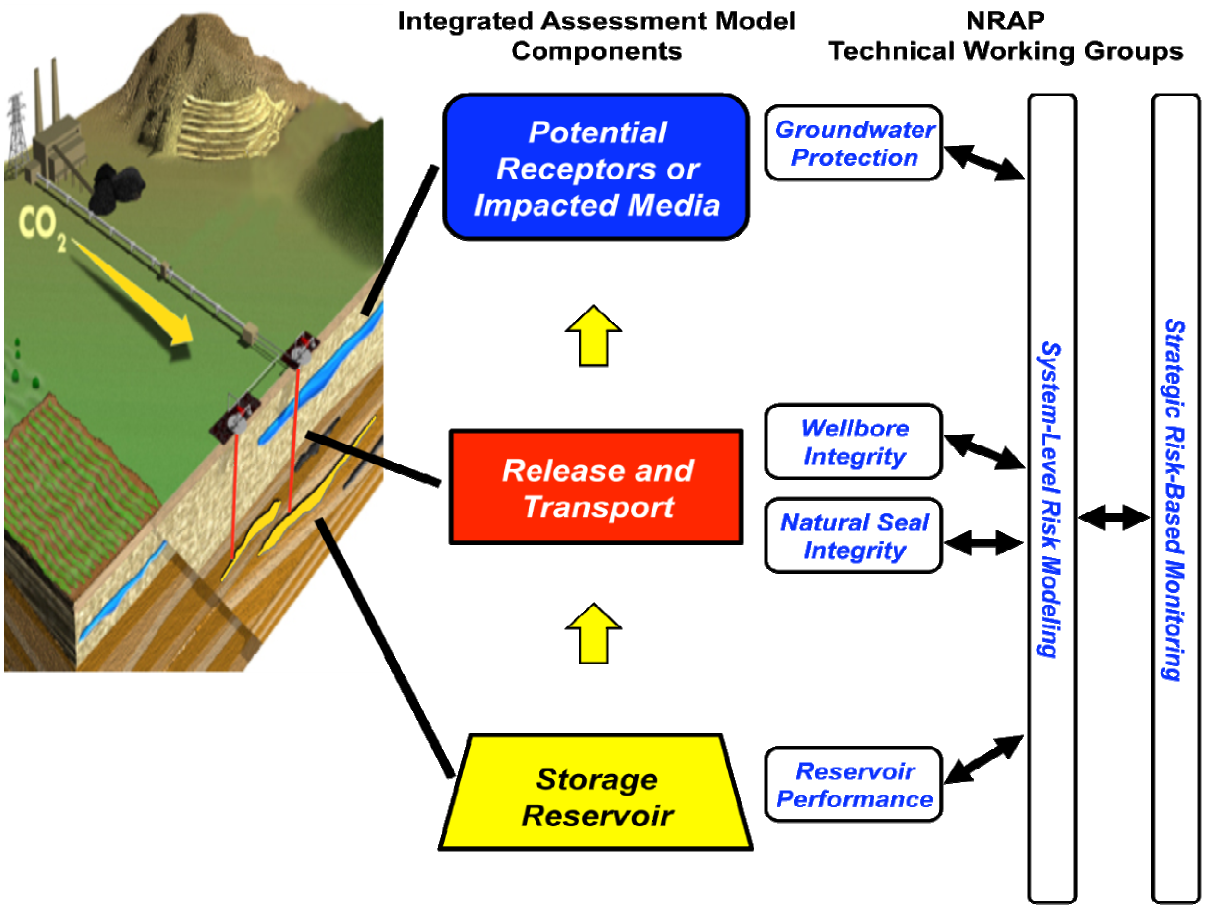

Figure 4.1: The integrated assessment model approach being used by NRAP and the associated NRAP technical working groups.

Once a methodology is developed, NRAP will work with field demonstrations (such as the Regional Carbon Sequestration Partnerships and other large-scale demonstrations) to apply it to real storage sites. NRAP also has plans to develop/exploit a variety of other field-based opportunities for obtaining data that allow quantification of system behavior and/or confirmation of the NRAP methodology.

5.0 Carbon Capture Simulation Initiative

The new DOE initiative on Carbon Capture Simulation was another modeling and simulation initiative briefly discussed during the Workshop. This initiative is a multi-lab simulation effort for accelerating the commercialization of carbon capture technologies from discovery to development, demonstration, and the widespread deployment to hundreds of power plants. The program will bring together the best modeling capabilities at NETL, LANL, LBNL, LLNL, and PNNL in partnership with academic and industrial institutions to develop a comprehensive, integrated suite of validated computational models for carbon capture technologies. Industry involvement will be a key component of this initiative so as to ensure that the computational tools being developed are both effective and of use by the end customers. The scientific underpinnings of the suite of models will also ensure that industry can maximize learning from successive technology generations or even competing technologies. The increased confidence in simulated designs obtained through this initiative will reduce the risk when incorporating multiple innovative technologies in a single new design, thereby accelerating the development cycle required to commercialize novel technologies.

Currently, new carbon capture technologies start either in a lab or a pilot-scale facility and slowly and incrementally grow into demonstration projects before being commercialized. This process can take 10-30 years. At the current pace of development, several decades will be required for the deployment of an effective and efficient Carbon Capture and Storage (CCS) technology because CO_2 capture systems substantially increase the complexity of power plants. Even the adoption of existing capture technologies is encumbered by a number of issues, such as scaling up by a factor of 10, the large footprint of the capture plant, major equipment modifications, availability of regeneration steam, deep sulfur removal, parasitic power load, and substantial increase in the cost of electricity. Nonetheless, DOE has set a goal to begin widespread, affordable deployment of carbon capture and storage technologies within 8 to 10 years.

Advanced modeling and simulation capabilities when validated by physical evidence, build confidence in technical decisions and have the potential to significantly reduce the time, capital, and operational costs of the development and deployment of novel carbon capture technologies. Recent modeling efforts demonstrate that simulations have the potential to allow rapid scale-up of technologies, thereby reducing or even potentially avoiding costly intermediate scale testing. New designs could be tested via simulations to guarantee reliable operation under a variety of operating conditions. The multi-lab partnership will develop a modeling and simulation software infrastructure that enables the acceleration of CCS technology development by:

- Identifying the most promising concepts to pursue by screening materials, devices and processes
- Developing optimal designs and tradeoffs between performance, cost and reliability goals by supporting the design and troubleshooting of devices and processes

- Quantifying the technical risk of the various steps in going from lab-scale to commercial-scale
- Stabilizing the costs quickly during deployment from the 1^{st} to the N^{th} plant by using virtual plant simulation to increase the rate at which understanding and knowledge are developed.

The Carbon Capture Simulation Initiative (CCSI) is different from ASCEM and NRAP; whereas ASCEM and NRAP focus on natural systems, CCSI focuses on engineered systems (specifically, carbon capture technologies for power plants). However, this does not preclude sharing new simulation technologies between the programs. One possible area of collaboration is the development of optimization and uncertainty quantification tools that would help the design process. These tools may be generic enough that new technologies developed within ASCEM and NRAP may be of use within CCSI and vice-versa.

6.0 Computational Platform Breakout Group

Both ASCEM and NRAP are designed to support not only risk assessment but also the basic process of iterative data collection, experimentation (laboratory and field), and numerical simulation to improve our understanding of the science underpinning complex subsurface systems. This iterative process forms the basis of a general decision-making process. Both projects are concerned with coupled thermal, hydrological, mechanical and chemical processes in a multi-fluid, multi-phase, multi-component setting. To predict the behavior of the integrated system, these projects must link together models for multiple compartments (sub-systems) that could potentially be governed by different underlying physics.

The iterative process encourages development of 'living models,' which continuously improve and provide better predictions as new knowledge and data are obtained. ASCEM and NRAP are using different approaches for providing a computational platform that integrates such knowledge and data:

- NRAP is utilizing either existing numerical codes (e.g. PNNL's STOMP, LBNL's TOUGH2, LANL's FEHM and LLNL's NUFT, etc.) or analytical/semi-analytical models for simulating coupled processes within individual compartments of the sequestration system, and the GoldSim systems-level modeling platform for linking multiple compartments.
- ASCEM is developing a new computational platform and a high performance simulator along with tools for parameter estimation, uncertainty quantification, decision support, data management, visualization and risk assessment. The ASCEM platform should provide a much more facile and responsive process for building models than those currently available. Although the 'legacy' simulation codes currently used at the national laboratories are capable of doing highly

detailed and powerful simulations, constructing models and evaluating their output can be quite burdensome.

The Computational Platform breakout group, identified five areas where opportunities may exist for collaboration and sharing results.

6.1 Uncertainty Quantification Tools

(a) Similarities and Differences

Both NRAP and ASCEM programs see a significant role for uncertainty quantification (UQ) tools and approaches. Within NRAP, there are two somewhat distinct roles for UQ. The first is within systems modeling, which forms the backbone of risk assessment. Each component of the systems model is associated with uncertain parameters; many randomized realizations must be generated and compiled into an integrated risk assessment with uncertainty. The second role for UQ is within the context of basic scientific investigations, when simulations are used to interpret lab and field data and to form predictions, and UQ is used to assess the adequacy of data and models to guide future investigations, including model refinements. At present, NRAP relies on UQ toolsets available within the Goldsim platform for specifying parameter distributions, running Monte-Carlo simulations and general UQ approaches.

ASCEM is developing a UQ toolset, which will provide a full suite of parameter sampling algorithms, global sensitivity analysis algorithms, predictive analysis tools, and constrained optimization tools to guide uncertainty reduction strategies. Tools for both low and highly parameterized models will be available. For models with significant calibration constraints, which impart non-linear dependencies between parameters, alternatives to strictly Monte Carlo sampling will be provided. Most of these algorithms have been developed elsewhere. The ASCEM UQ toolset will be integrated with a decision support toolset.

Both NRAP and ASCEM recognize the importance of considering not only parametric uncertainty but also conceptual model and scenario uncertainty. This requires new algorithm development and ASCEM intends to invest in this area.

(b) Recommendations

It may be instructive to compare the suite of 'standard' UQ tools/approaches currently implemented by NRAP and the first set of UQ tools implemented in ASCEM for the December, 2010 demo. A possible outcome of this comparison would be for the NRAP algorithms to be added to the ASCEM UQ toolsets, or vice-versa. As new approaches for addressing conceptual model uncertainty are developed as part of the ASCEM project, these tools/approaches will be available to NRAP researchers. Feedback on their applicability from the NRAP scientists will benefit the ASCEM project.
NRAP is especially interested in taking advantage of ASCEM algorithms designed to address uncertainty quantification if parameters are correlated. Other than the trivial case of linear correlation, this situation can cause Monte Carlo sampling strategies to produce very unrealistic model outcomes. As soon as ASCEM integrates these tools in the UQ toolset, the capability will be shared with NRAP colleagues for testing and feedback.

NRAP will also be performing UQ analysis as part of the risk profile quantification process. The approaches/algorithms utilized within this context will be shared with ASCEM for feedback.
Hold a joint meeting on lessons learned on UQ analysis following ASCEM's December 2010 demo.

6.2 Approaches for Model Reduction and Response Surfaces

(a) Similarities and Differences

For the purposes of risk assessment, parameter estimation, or uncertainty quantification, many realizations of a single model will be necessary within both ASCEM and NRAP. Detailed coupled-process models may have long run-times which may not afford large numbers of runs. For this reason, simplified models (reduced dimension, reduced grid resolution, reduced number of processes, weaker coupling, etc.) or response surfaces may be developed.

(b) Recommendation

NRAP will be developing approaches for model reduction and response surfaces to incorporate into Goldsim within the context of risk profile calculations. ASCEM plans to offer utilities for developing such models with steps that include facile development of reduced model(s) or response surfaces and evaluation of errors incurred by the simplification.

NRAP and ASCEM will share approaches developed by either project. The abstraction strategies used by NRAP will be available to ASCEM for incorporation in the platform. The ASCEM utility toolset for developing such models will be available to NRAP scientists for testing and feedback.

Hold a joint meeting on lessons learned and sharing approaches taken for model reduction following NRAP's risk profile calculations in FY11.

6.3 Data/Knowledge Management & Integration

(a) Similarities and Differences

Both NRAP and ASCEM are interested in approaches that efficiently capture new scientific understanding and processes/models within the risk assessment process. Additionally, for both projects it is important to provide a consistent, readily accessible, and transparent repository of data, knowledge, and models as well as simulation results. This will require the following:

- A searchable repository to browse and share data/knowledge within a project context (e.g., goal, experimental data, characterization, derivation information, etc.)
- Capturing provenance of site data, model parameters and model inputs and outputs

- A consistent repository of the technical basis (e.g., data, reports, logs, scripts, etc.) for conceptual models, simulator inputs, and outputs
- Translation of conceptual models to simulator inputs
- A user interface to facilitate data/knowledge input, sharing, retrieval, and application in simulation, uncertainty quantification, risk assessment, and decision support.

While the attributes related to data provenance are, in general, important for CO_2 sequestration risk assessment, they are not as critical to the current NRAP project scope as they are to the ASCEM program regulatory scope.

(b) Recommendations

While NRAP is interested in tools/approaches for efficient management and integration of data and knowledge, explicit development of such tools is not currently a high priority. On the other hand, ASCEM will be actively developing various tools/approaches for this purpose. As ASCEM progresses, a number of opportunities will become available for sharing tools, exchanging ideas with, and soliciting feedback from NRAP. A short-term opportunity will be related to the GS3 platform developed specifically for CO_2 sequestration application but modified for ASCEM application.

We recommend the following:

- Share basic ASCEM platform functionality and early release knowledge management tools based on GS3 with NRAP by the end of FY11 first quarter
- Obtain NRAP review and input on ASCEM platform requirements to identify specific functionality that may facilitate future development and application for carbon sequestration by the end of FY11 second quarter
- Share ASCEM FY11 platform demonstration results and lessons learned, including initial release data management approach and tools following the December 2010 demonstration
- Leverage cross-fertilization of NRAP and ASCEM teams to facilitate information sharing as programs advance.

6.4 Transparency and Traceability

(a) Similarities and Differences

It is essential to both NRAP and ASCEM that regulators and stakeholders have confidence in the technical bases and model results that support decisions. This means that the process must be transparent and provide a means to trace results back to the data used to produce them. Such transparency and accountability will also support making sound and scientifically defensible decisions to manage/minimize risks. An effective approach to do this will:

- Utilize provenance of data, parameters, model inputs, etc. to understand what has been done, trace impact of changes in data and models

- Provide readily accessible information on basis of model input and results (e.g., transparency)
- Provide a historic record of the technical basis used to support decision making
- Assure repeatability of model inputs/parameters and tracking of model and simulator versions

(b) Recommendations

While NRAP is interested in tools/approaches that improve transparency and traceability, such tools will not be explicitly developed within the overall scope of the NRAP project. On the other hand, NRAP will be publicly sharing the results, models, and approaches developed during the project with the broader community. As part of its work scope, ASCEM will be developing tools/approaches for data provenance, document tracking and quality control. As these developments become public, such as tools included in GS3, there will be opportunities for sharing information.

We recommend sharing ASCEM methodology for providing open/community access and sharing of data, models, and results to facilitate knowledge management. The existing knowledge management tools in GS3 could be shared now (as they are for the Sim-SEQ effort within the regional carbon sequestration partnerships), followed by broader ASCEM tool sharing in FY12.

6.5 Visualization Approaches

(a) Similarities and Differences

For better communication as well as effective decision-making, both NRAP and ASCEM will need tools for effectively visualizing data/results of various types and complexities. Central to both projects are geologic systems, which can be complex and heterogeneous. In addition, the risk assessment goals of both projects will require tools to effectively communicate multi-dimensional, probabilistic results.

(b) Recommendations

NRAP is planning on utilizing currently available visualization tools, including those provided by the GoldSim platform for probabilistic assessment. ASCEM is developing novel visualization methods for exploring large-scale model outputs and supporting uncertainty quantification and decision support activities. As these visualization tools are developed, they can be made available for NRAP to explore and utilize.

We recommend sharing ASCEM developments for novel visualization tools with NRAP. The earliest opportunities for this are likely to be in FY12 after the release of the first version of the ASCEM toolset.

7.0 Verification & Validation/Model Confirmation Breakout Group

In this breakout session, participants discussed the methods and means by which models can be used iteratively with measurements and testing to reduce uncertainty associated with risk-assessment for CO_2 sequestration (NRAP) and legacy waste (ASCEM). Participants in this breakout session discussed the types of risk assessments performed in each program, and examined the similarities and differences in each program, as well as potential initiatives that could be leveraged to maximize efficiencies and promote common practices.

A major effort and accomplishment in the breakout session was ensuring that each project group gained an appreciation of the goals and approaches of the other. As an initial outcome, the participants agreed to a definition and preferred term to define the process of integrated model-experimental studies: "model confidence building." This term, while less definitive than verification and validation (V&V), properly reflects the process whereby a model is gradually improved (i.e. a living model), vetted with interested parties, and ultimately deemed to be appropriate for use in performing risk assessment analyses.

As an organizing concept, Figure 7.1 outlines a systems approach for risk assessment in which model development is an integral component that is tested and refined with data to reduce uncertainty. In the figure, lab or field-based testing, which provides the underpinning data that is required to build confidence in a model, is defined in the context of a specific CO_2 sequestration site or a contaminated field site. Two types of uncertainty are generally present: conceptual model, and parametric. An experimental and observational program integrated with a model development effort is required to reduce these uncertainties. Conceptual model uncertainties stem from lack of knowledge of the fundamental controlling physical/chemical processes, initial conditions, and boundary conditions that apply in a given field situation. Even when the conceptual model is well established, the appropriate model parameters that apply at the site may be uncertain, and limited by sparse data. This is parameter uncertainty.

As illustrated in Figure 7.1, field test or site characterization data are tightly integrated with a field test model to provide a continuously updated assessment of uncertainty in parameters and models. These uncertainties, derived from the testing analysis and site characterization information, are applied to predictions of system performance for the risk application of interest. Risk projections are vetted with decision makers and technical peers at regular intervals, leading to refinements of the testing program. In this manner, uncertainties, and ultimately risk, are systematically reduced to acceptable levels. The field test model is often based on a controlled field experiment designed to reduce conceptual or parametric

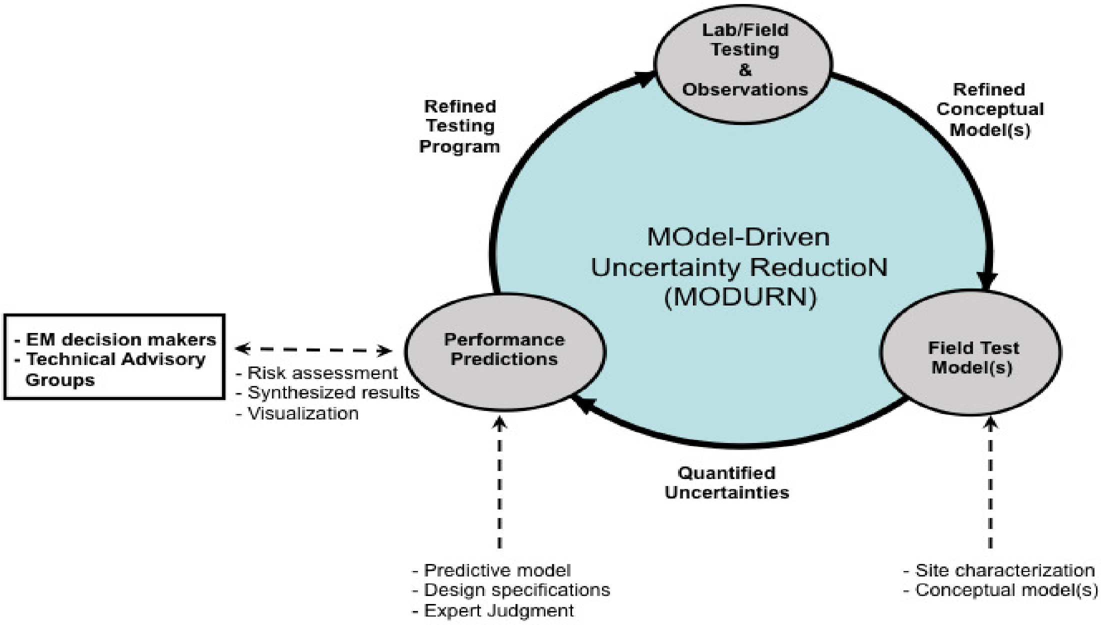

Figure 7.1. Schematic of the Model-Driven Uncertainty Reduction paradigm.

uncertainty rather than a model of the entire site. Although the term “validation” or “model confirmation” can be applied to this model, ultimately the risk predictions, which apply to the site as a whole, are of greatest concern since they will be used to make decisions on remediation or monitoring plans, or the disposition of license applications. In addition to the information from field test models, basic characterization data, and data on items like contaminant observations or measurements of system response to CO_2 injection are all used to develop the predictive model (labeled “Performance Predictions” in the Figure 7.1).

Ultimately, we would hope to create a process in which risks are continuously updated based on available data. However, most real situations do not approach this limit, with models generally lagging behind data collection and testing. In this session, we described the ways in which each program is attempting to use modeling and data collection to reduce the cycle time required to complete the characterization-testing-prediction loop.

The next two subsections explore the methods by which each program is using experimental scientific studies to aid in the process of model confidence building.

7.1 ASCEM Approach to Model Confidence Building

In ASCEM, the Site Application Thrust is overseeing the modeling of several demonstration sites to build confidence in models and approach, and to engage the site user community. These sites will provide data for model development and testing, and provide linkage between the computational capabilities and specific DOE-EM sites that require advanced modeling. A key benefit of this approach is that it helps to establish and maintain linkages with end users. The Site Applications Thrust will also provide feedback for developing the HPC and Platform components of ASCEM based on user experience, as well as disseminate information and provide training.

Initial efforts have focused on developing a list of candidate sites and/or environmental problems that could be used for demonstrating ASCEM capabilities. The leaders of this effort have followed an organized process, including establishing the criteria and metrics for selecting sites. To maximally exploit ongoing scientific efforts, sites/problems considered include all of the Office of Science IFRC and EM Applied Field Study Sites as well as other interesting and DOE-relevant problems. From this systematic process, the project decided that the focus of the Phase I (2010) demonstration would be the Savannah River Site (SRS) F-Area (Figure 7.2). In addition, the ASCEM development team may also consider tackling aspects of two other sites/problems during 2010, including the Hanford Deep Vadose Zone and a Tank Waste Performance Assessment problem. Phase II demonstrations (2011) will definitely include these three areas in addition to defining a demonstration focused on the mercury contamination at Oak Ridge.

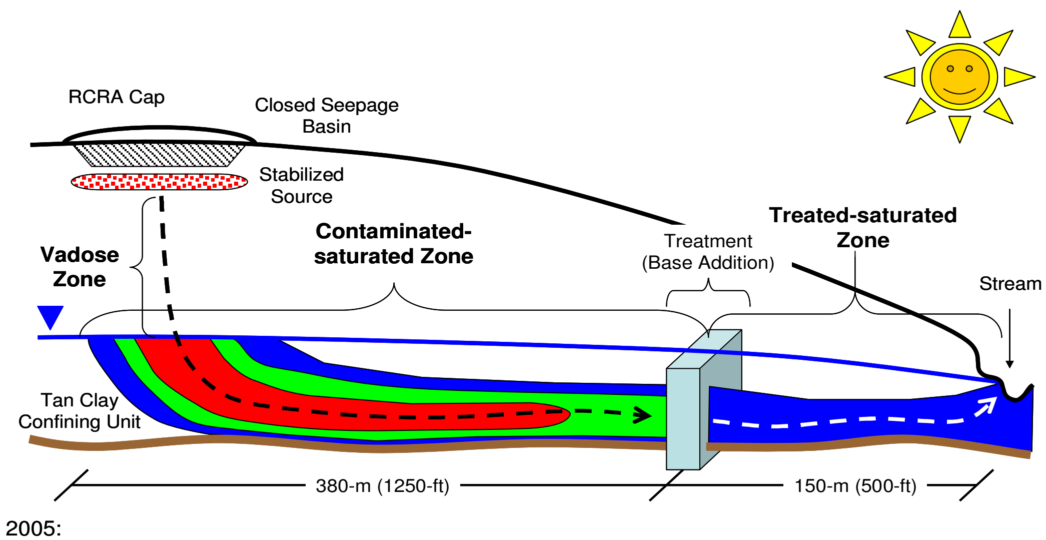

Figure 7.2. Conceptual model of the Savannah River F-Area Groundwater Plume

A brief description of the Savannah River F-Area site application project follows. The SRS F-Area was the location of a seepage basin that resulted in an acidic groundwater plume containing U and other contaminants (Figure 7.2). It is a priority site for DOE, where a variety of enhanced and long term monitored natural attenuation (MNA) research and technologies are being advanced with support from EM-32 (to SRNL) and BER (LBNL SFA). It is being designated as an EM-32 Applied Field Research Center. Currently, a funnel-and-gate system with base injection is operating at the site to neutralize groundwater and thus immobilize U down gradient of the seepage basins. The conceptual model of MNA at the site is that rainwater will eventually neutralize the lingering mineral surface acidity, causing an increase in pH, which may naturally immobilize U in the trailing end of the plume. If the natural pH neutralization up gradient from the treatment system is insufficient, additional enhanced neutralization will be required up gradient and/or in the vadose zone. Critical to assessing the in-situ treatment requirements over the long time frame is the development of an understanding of the long-term H^+ and U sorption behavior at the site.

The Phase 1 Demonstration will highlight various components of the ASCEM high performance computing and platform infrastructure. The focus during the first year will be in four major areas: 1) High Performance Computing, 2) Visualization, 3) Data Management, and 4) Uncertainty Quantification. The components will be tested individually using site data, with the goal of integrating these components in 2011. An F-Area ‘working group’ will be responsible for 1) evolving the direction of the ASCEM demonstrations, 2) assembling the necessary input (conceptual models, data, process models, and other expert input) needed for ASCEM demonstrations, 3) working closely with the developers to advance and test ASCEM capabilities using realistic and relevant datasets, and 4) engaging potential end-users in the development and use of ASCEM.

7.2 NRAP Approach to Model Confidence Building

Ensuring that large-scale CO_2 storage is safe and effective requires predicting the long-term integrity of storage sites as well as demonstrating the comprehensive consideration of potential site-specific risks. In addition, quantification of the likelihood of these risks is an integral component of both assessing potential long-term liability, and designing site-specific monitoring and mitigation strategies to minimize risk. A strategic integration of monitoring and mitigation with risk assessment can also lower both uncertainties in predictions, and risks overall.

The scale of CO_2 storage sites makes science-based prediction over these large sites challenging. An individual storage site may have a footprint on the order of 100 km^2, and the need to consider the behavior of the site’s system from the reservoir to potential receptors results in a large volume that must be addressed in the predictions. Further, widespread commercial deployment will necessarily require the consideration of a large number of sites spanning a range in geologic diversity. Finally, the complexity and heterogeneity of natural systems imparts a degree of uncertainty and complexity onto any predictions, necessitating a stochastic component to the methodology. These complexities underscore the importance of integrating strategic monitoring with the predictions to reduce uncertainties while verifying that a site is performing as anticipated. Nevertheless, prediction of site performance as part of risk assessment remains challenging and will require a new set of science based tools that are validated to the extent possible on observations from natural systems.

Comparison of the predictive methods against observations is critical to demonstrate reliability and accuracy as well as to reduce uncertainties. Data from Regional Carbon Sequestration Partnership (RCSP) field demonstrations provide critical observations for early stages of operation. Observations relevant to long-term stewardship will require analog field sites (e.g., industrial sites and natural sites like CO_2 reservoirs, CO_2-rich gas reservoirs, etc.). Exploitation of opportunities from RCSP projects and other large-scale field demonstrations is part of the strategy NRAP will use to develop the data necessary to build a complete understanding of key processes that impact risk associated with CO_2 storage as well as the data necessary to confirm the NRAP predictive methodologies. NRAP will also conduct additional field efforts as necessary, targeting key data gaps (particularly those associated with long-term processes that develop, at times, scales beyond the reach of RCSP efforts).

The NRAP program evaluates the fundamental mechanisms associated with the release of injected CO_2 or other formation fluids from a CO_2 sequestration site. The organizing concept is the risk profile, shown schematically in Figure 7.3. This risk profile considers the storage reservoir, the mechanisms and pathways by which fluids might leak, and the consequences of such leakage. Pathways include the injection wellbore or other wellbores drilled into the reservoir, and geologic pathways (such as fractures and faults) through the natural seals that otherwise provide integrity and long-term isolation of the CO_2 from the overlying strata. Potential receptors include an overlying groundwater aquifer and the atmosphere above the ground surface. Additionally, the possibility of induced seismic activity in the form of ground motion is being considered.

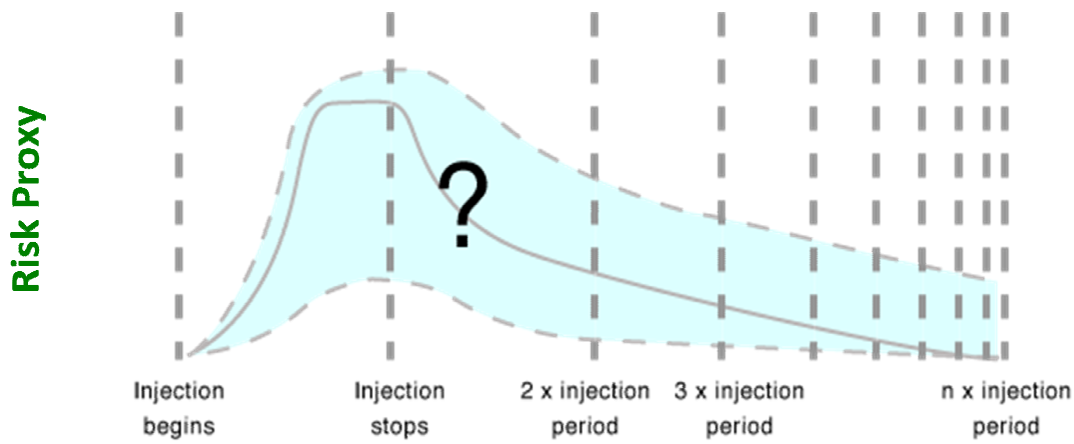

Figure 7.3. Schematic of risk profile for CO_2 sequestration that will be developed on a site-specific basis to calculate residual liability for long-term stewardship.

A comprehensive treatment of this system requires that the fundamental processes associated with the reservoir, the leakage pathways, and the response of the receptors to CO_2 intrusion be understood. The NRAP program has a comprehensive scientific program designed to do the underpinning science needed to build confidence in the models used in the risk assessments. One of the key receptors being investigated is the impact of CO_2 leakage on drinking water quality. Risk proxies that have been identified include the pH and total dissolved solids (TDS), which may be impacted by the intrusion of CO_2 or brine into the aquifer. Preliminary modeling analyses have been performed using reactive transport codes to assess the geochemical response of an aquifer to leakage over a prescribed period of time.

Accurate prediction of the impact of leaking CO_2 or reservoir fluids on groundwater quality is limited by the complexity of subsurface aquifers and the geochemical reactions that control drinking water compositions. As a result, there is a high uncertainty associated with any prediction, hampering monitoring plans, interpretation of the monitoring results, and mitigation plans for a given site. A key focus of NRAP is to quantify the uncertainty to groundwater quality impacts predicted from combined field and laboratory data. One planned activity, subject to approval and agreements between the parties, is a controlled CO_2 release experiment in a shallow aquifer, intended to evaluate the consequences of CO_2 intrusion from a deep storage operation. If this work goes forward, it will provide a unique opportunity to define and reduce the uncertainty on groundwater impacts by using state of the art uncertainty quantification techniques, high performance computing techniques, and monitoring data. This work would augment the existing experimental and reactive transport simulations. NRAP participants will work with monitoring data collected by the research teams involved in this project, to the mutual benefit of both parties.

Similarities and Differences in Approaches to Model Confidence Building
The breakout session discussion identified several areas of common need for the ASCEM and NRAP programs. To frame the discussion, it is convenient to first discuss the differences. At a high level, the performance or risk assessments (ASCEM) and risk profiles (NRAP) both rely on underpinning experiments and observations to build confidence in the models. However, the NRAP goals have several system components that are not directly relevant to ASCEM, including pressure and geomechanical effects in the storage reservoir, and the interaction of CO_2 with wellbore cement. Conversely, the ASCEM focus on contaminate transport has some, but not strong overlap with NRAP.

From the perspective of environmental systems, the area of greatest overlap is contaminant migration in groundwater. For ASCEM, both unsaturated and saturated porous media are relevant, whereas NRAP's focus is the mobilization of metals, radionuclides, and other dissolved constituents in saturated groundwater flow. Both programs deal with confirmation of conceptual and numerical models of dissolved species transport, and both deal with the issues of detection and monitoring.

At a more conceptual level, the issues of up-scaling are common to both programs. There is a need to develop robust methods to take experimental information from the laboratory and small field scale to a much larger scale relevant for risk assessments. Another aspect of up scaling is the need to place field measurements, with a "support scale" of perhaps a few cubic meters, in a large-scale context. The question of how best to incorporate small-scale measurements into a large-scale model is an open research question relevant to both programs. In addition, both programs need to build uncertainty quantification into the field investigations being contemplated. Uncertainty is a given, regardless of the level of investigations performed, so an effective means for quantifying conceptual and parameter uncertainty, and driving these uncertainties lower over time, is a critical component of model confidence building.

7.3 Opportunities for Collaboration in Model Confidence Building

The opportunities for collaborative work by the two programs fall into a broad range of activities in what can be called "uncertainty quantification in practice." By this we mean that in each program, there are activities in which laboratory and field-scale efforts are needed to rigorously understand the controlling processes in an actual field setting, and to quantify uncertainties in both model conceptualization and in terms of parameter uncertainties. The goal in each case is to demonstrate improved scientific understanding, and to provide real-world examples of how the model-driven uncertainty reduction process depicted in Figure 1 can be implemented.

Given that the field applications being promoted in the two projects are specific to the needs of the project, the breakout session participants believe that the most fruitful type of collaboration would be to have regular technical exchanges to share best practices. In these technical exchanges, the ASCEM Site Application effort and relevant aquifer groundwater impacts field investigations (such as the EPRI experiment) conducted in NRAP would be presented, with the exchange centered on the technical issues surrounding the implementation of the model-driven uncertainty reduction method (Figure 5.1). Focusing these exchanges in the area of greatest technical overlap (geochemical transport in groundwater) of the two programs maximizes the likelihood of meaningful dialogue and lessons learned. Likely topics in these technical exchanges are:

- Geochemical transport numerical model formulations
- Treatment of conceptual model uncertainty, including uncertainty in geologic structure, boundary conditions, etc.
- Desired level of model complexity
- Model reduction: development of reduced order models
- Up-scaling methods, treatment of heterogeneity
- Incorporation of field data into models
- Using decision support tools, optimize monitoring and field measurements
- Use of decision support tools.

Beyond the groundwater geochemical transport application, chemical behavior and stability of cement was identified as another area in which technical exchange could be beneficial. It is recommended that subject matter experts in the two programs meet to discuss common issues and approaches. Finally, it is recommended that the two programs jointly develop a list of experimental capabilities (laboratories, equipment, field deployment capabilities) that are present at the National Laboratories in areas of relevance to the programs to ensure the maximum level of awareness of management of the available capabilities.

8. Multi-Physics HPC Simulator Breakout Group

The purpose of this breakout session was to flesh out the commonalities and differences between the multi-physics couplings that are needed for ASCEM and NRAP, and to evaluate leveraging and coordination between the programs in the area of multi-physics HPC simulators.
To establish common terminology for the discussion, we began by clarifying our working definitions of both multi-physics and High Performance Computing (HPC).

The term multi-physics is commonly used to capture the important concept of coupled processes, including hydrological, biogeochemical, geomechanical, and thermal processes that may be relevant to both ASCEM and NRAP. Within ASCEM, this has been dubbed multi-process coupling to reflect a breadth that goes beyond traditional physics.

In contrast, the multi-faceted meaning of the term High Performance Computing, which is commonly referred to by its abbreviation HPC, may be less intuitive. Specifically, the important facets of HPC for this breakout session include:

- Advanced or state-of-the-art numerical algorithms providing flexibility, robustness, and fidelity that were likely unavailable 10-15 years ago.
- Algorithms and implementations designed for parallel systems, ideally taking advantage of emerging petascale computational facilities.
- Implementations that leverages advanced HPC Frameworks (such as Trilinos and PETSc) along with modern object oriented design concepts.

It is from this viewpoint that ASCEM is developing its Multi-Process HPC Simulator.

8.1 Multi-Physics HPC Simulations

One of ASCEM's core tasks is the development of a new flexible and extensible HPC simulator for the prediction of contaminant fate and transport processes relevant to DOE-EM's mission (the third thrust area as introduced in Section 3). The computational engine will be designed as modular and open-source, with the ability to handle various relevant coupled processes (i.e., multi-physics). It will run on platforms ranging from laptops to emerging petascale computers. To achieve this, ASCEM will leverage the considerable scientific investments both within and outside of DOE-EM to better understand the science of complex environmental systems. Thus, ASCEM'S HPC Simulator Thrust can concentrate on the development of the computational engine for modeling multiphase, multicomponent, multiscale subsurface flow and contaminant transport, and cementitious barrier and source-term degradation, while relying on a scientific understanding of processes and couplings derived from integrated research activities funded elsewhere.

NRAP's core mission is to develop a defensible, science-based, quantitative methodology for determining long-term risk profiles at CO_2 storage sites. This requires 1) that system-level risk assessment methodologies are developed and applied, and 2) that key scientific gaps and uncertainties in understanding such complex systems are being addressed through an integrated experimental (laboratory and field experiment) and simulation approach. While multi-physics computational engines such as ASCEM's new HPC simulator would be beneficial in achieving NRAP's goals, the program currently focuses its resources on these two requirements, utilizing the multi-physics simulation capabilities currently existing within the DOE complex (such as LBNL's TOUGH family of codes, LANL's FEHM and PFLOTRAN, PNNL's STOMP, and LLNL's NUFT). These existing simulators have been applied widely within the CO_2 storage community. They address many of the relevant multi-physics and coupling requirements, however, they have varying degrees of computational efficiency and limited applicability to emerging multi-core computer architectures.

8.2 Similarities and Differences in Approaches to HPC Simulations

Participants in the multi-physics HPC simulator breakout group agreed that both programs would benefit from a flexible, best-in-the-class computational engine such as the one being developed within the ASCEM program. Important reasons to exploit HPC resources common to both programs include:

- Enhances fidelity of solutions allowing for complex couplings and higher-resolution modeling of subsurface heterogeneity
- Provides robust and modular design to enable the flexibility in the development of conceptual model hierarchies to fully explore uncertainty quantification and attribution
- Enables UQ/optimization/sensitivity/inversion approaches that may involve thousands of individual forward runs and it may enhance or accelerate these studies through more intrusive features, such as the direct computation of forward and adjoint sensitivities
- Allows system-level modeling with more complex multi-physics processes in lieu of limiting assumptions and abstractions
- Allows modeling of multi-physics processes occurring over a range of spatial scales from pore-size to basin-scale, for time periods ranging from several hundred to thousands of years.

A typical NRAP simulation example in support of risk assessment for CO_2 storage sites is the long-term prediction of CO_2 plume migration and trapping. In industrial-sized storage projects, the plume of supercritical CO_2 may extend 10 to 20 km from the injection well, but its flow behavior is determined by microscale physics within the rock pores combined with medium- to large-scale geological heterogeneity. In the longer term, the CO_2 can gradually dissolve into the ambient salt-rich aqueous fluids in the rocks. This process produces a dense, mixed fluid that will sink due to negative buoyancy rather than rise as pure CO_2 does. Finally, on time scales that extend to 1000's of years, the CO_2 can chemically combine with Ca, Mg, and Fe to produce carbonate minerals that partially fill the pore space, a process that results in permanent storage of CO_2. Such complex system modeling of coupled processes over a vast range of spatial and temporal scales can be a challenge to currently existing simulation codes.

It was suggested in the breakout discussions that both programs could benefit from a "common architecture at many sites" paradigm in which standardization of software, methods, and approaches is promoted by developing a risk assessment framework that can be applied to multiple sites. Among other advantages, regulators value standardization and accountability across different projects. It was pointed out, however, that the many different stakeholders in the CCS community (R&D, oil and gas industry, energy companies, regulators, NGOs, etc.) use a wide range of open-source and proprietary simulators and may not wish to transition to another. NRAP currently plans the development of a standardized methodology for quantitative risk assessment, but for the near-term they will use existing computational engines to evaluate the underlying multi-physics simulations.

While NRAP does not necessarily require a new “best-in-the-class” HPC simulator to achieve its application-driven mission, the program and the CO_2 community at large have expressed that such a tool is desirable, and in this case, could leverage ASCEM's achievements as a starting point for HPC computations of risk-relevant processes in CCS projects. As it is designed, ASCEM's HPC simulator will be a flexible, extensible and versatile tool, allowing introduction of additional processes and couplings in a straightforward manner. ASCEM and NRAP share the need for multicomponent, multiscale simulations of flow and reactive transport in natural subsurface environments, and in the performance of cementitious barriers (i.e., tanks in DOE EM's complex, wellbore cements in CO_2 applications). There are, on the other hand, fundamental differences in the importance of physical processes to be considered, as well as in the level of coupling between processes. For example, NRAP requires a stronger emphasis on true multi-phase systems (water, CO_2, and/or oil and gas) and phase transitions, and a stronger emphasis on geomechanical coupling and non-isothermal effects. NRAP also requires handling a much larger range of subsurface pressure and temperature conditions. Extension of ASCEM's HPC simulator for CO_2-related purposes will be feasible once a prototype version exists in a couple of years, but it will require modifications and additions to currently planned simulator capabilities

8.3 Recommendations

Breakout participants recommended a sequenced approach to ensure coordination and potential leveraging between ASCEM and NRAP with respect to multi-physics HPC simulations.

(a) Short-term Recommendation (Second quarter FY11):

- Conduct regular information exchanges toensure communication/sharing of data between the two programs via regular meetings of leadership teams, or via participation of NRAP representatives in ASCEM progress meetings, and vice versa.

(b) Mid-term Recommendation (End of FY11):

- Communicate NRAP process modeling requirements to ASCEM leadership team
- Develop a document describing the NRAP-CO_2 process requirements that are different or additional to ASCEM's process requirements
- Define a suite of NRAP-related simulation test cases which can be added to ASCEM's list of benchmarking problems

- Using the above, ensure that ASCEM design of the multi-physics HPC simulator is not too restrictive for possible future use in NRAP (i.e., solicit regular NRAP community input, including potential NRAP participation in ASCEM internal code review).

(c) Long-term Recommendation (Next 2-3 years):

- Develop a staged approach for extension of ASCEM's multi-physics simulator to accommodate NRAP requirements.
- A decision on close integration of ASCEM and NRAP should be made after both programs have reached sufficient maturity.
- ASCEM extension and application to NRAP problems should start with low-hanging fruit, possibly addressing some, but not necessarily all of NRAP's modeling needs.
- Early applications should be CO_2-related problems that can be solved by ASCEM's computational engine without major additions (e.g., reactive transport in groundwater in the event of CO_2 leakage).
- Capabilities should be added to ASCEM's computational engine in a staged manner, starting with those that require minimum effort and offer maximum benefit (e.g., starting with multi-phase capabilities to allow for HPC reservoir modeling, followed by non-isothermal processes, followed by geomechanical coupling).

9. Summary of Overall Conclusions

Undersecretary Christina Johnson noted that computational modeling and simulation are at the core of several new program initiatives within DOE-EM and DOE-FE, and requested of Assistant Secretaries, Inés Triay and Jim Markowsky, to convene a workshop to investigate potential synergy between DOE-EM's Advanced Simulation Capability for Environmental Management (ASCEM) and DOE-FE's National Risk Assessment Program (NRAP) initiatives. These two initiatives are aimed at providing science-based predictive modeling approaches for better risk assessment understanding of the challenging problems facing DOE in subsurface contaminant transport, and carbon capture and storage. More broadly, the topic of flow and heat and mass transport in subsurface media has broad applicability across the spectrum of energy initiatives within the Department, including nuclear waste disposal, environmental stewardship (including nuclear waste disposal), engineered geothermal systems, environmentally sound and efficient production of fossil fuels (both conventional and unconventional), geological storage of CO2, and management and production of water resources. Decisions in each of these areas require advanced predictive capabilities that can quantify accurately the behavior of natural systems resulting from coupled physical processes (e.g., multiphase flow, heat/mass transport, biogeochemical reactions, and geomechanical responses) that occur over multiple length and time scales in natural systems (whose properties are inherently heterogeneous and uncertain). Future challenges will require the integration of new computational tools with new observations on the behavior and properties of geomaterials and geosystems. DOE has two new initiatives building aspects of this new predictive capability in the context of science-based risk assessment for environmental stewardship and for geologic storage of CO_2.

A workshop was held September 1st and 2nd, 2010 to facilitate leveraging and coordination between DOE-EM's ASCEM and DOE-FE's NRAP initiatives. The ASCEM and NRAP initiatives are both DOE funded efforts designed to enable science-based risk assessment methodologies using best-in-class computational methods to integrate theory and observations. ASCEM is focused on developing a next-generation HPC simulation platform for environmental management, whereas NRAP is focused on developing a science based methodology for quantifying potential long-term risk (and, hence, liability) for geologic storage of CO2. As such, the two efforts address distinct energy challenges. Nevertheless, there is potential for synergy between the efforts. Both of these programs will focus R&D efforts on improving computational models and methodologies and quantifying uncertainties to uncover the most important knowledge gaps associated with the long-term fate and transport of fluids and chemical species in the natural environment, from surface waters to the subsurface. Given these similarities, the workshop participants (representing key technical and programmatic leads from each initiative) discussed the commonalities and differences that emerge when these high-level goals are applied in two distinct application areas: groundwater and soils remediation and long-term geologic storage of CO_2. The overarching goal of the workshop was to ensure integration and coordination across these two important national programs.

The ASCEM program is accomplishing its mission by developing a new state-of–the-art high performance computing capability and computational platform. The NRAP program is building on existing best-in-class computational tools and capabilities to meet its near-term program needs while focusing efforts on improved predictive descriptions for key processes. Both approaches will develop and use formal uncertainty quantification methods to direct their R&D efforts.

The use of higher fidelity, science-based models will build confidence in the risk assessment for engineered and natural systems. In both programs, systems-level models composed of submodels of individual components are required to link source terms, engineered and natural components, and receptors. The computational platform ASCEM is developing will be an open-source, community code that is flexible and able to exploit computers from the desktop to the HPC scale. For reasons of cost, efficiency, reliability, and credibility, each program has adopted a "common architecture at many sites" paradigm in which standardization of software, methods, and approaches is promoted by developing a system that can be applied to multiple sites.

Both the ASCEM and NRAP programs are at the beginning stages of ambitious 5-year research plans. As such, it makes sense to coordinate efforts in both programs so as to ensure maximum integration wherever possible in the long-term. Based on information collected during breakout sessions at the workshop, a summary of the main areas where collaborations are possible between the two programs and recommendations for future action are listed below.

Recommendation 1

Establish a regular dialogue between SC/BER, FE/NRAP and EM/ASCEM DOE management through regular interactions and sharing/review of products developed by each program.

Recommendation 2

A common theme throughout the workshop was the establishment of regular joint technical exchanges between the programs to share information. These exchanges would initially focus around the following areas of common work scope:

- Compare the suite of 'standard' UQ tools/approaches currently implemented by NRAP and the first set of UQ tools implemented in ASCEM for its December 2010 demo (The concept of model driven uncertainty reduction would be refined as both programs develop tools.)
- Model reduction and response surface generation within the context of risk profile calculations both programs are performing
- Specific tools/approaches for efficient management and integration of data and knowledge, such as the GS3 platform
- Sharing of methodology for providing open/community access to and sharing of data, models, and results to facilitate knowledge management
- Share developments for novel visualization toolsets being developed by ASCEM.
- Share best practices on the technical issues surrounding the chemical behavior and stability of cement.

These technical exchanges should be held on a bi-annual basis and begin during the second quarter of FY11.

Recommendation 3

Leverage cross-fertilization of key staff working on both the NRAP and ASCEM teams to facilitate information sharing as programs advance.

Recommendation 4

Begin development of a staged approach for extension of ASCEM's multi-physics simulator to accommodate NRAP's future requirements (e.g., starting with multi-phase capabilities to allow for HPC reservoir modeling, followed by non-isothermal processes, followed by geomechanical coupling). This will be done in a stepwise fashion:

- Communication of progress and sharing of ideas though the technical exchange process listed in Recommendation #1

- Use these technical exchanges to communicate NRAP process modeling requirements to ASCEM leadership team for incorporation into the long-term development of the ASCEM HPC simulator
- Define a suite of NRAP-related simulation test cases which can be added to ASCEM's list of benchmarking problems on the HPC simulator.

Recommendation 5

Based on the workshop's success, it was recommended that similar focused "bilateral" workshops be conducted between ASCEM and other programs conducting subsurface science research. This would maximize opportunities to fully educate other DOE Offices on ASCEM's capabilities to address critical DOE missions (e.g., repository science through a combined Office of Environmental Management and Office of Nuclear Energy (EM-NE) workshop, and surface water/groundwater hydrology through an Office of Environmental Management and Office of Science (EM-SC) workshop).

Appendices

10. Appendix A: Workshop Agenda

Agenda ASCEM/NRAP Workshop
DOE Complex Germantown, MD
September 1st , 2010

Germantown Auditorium (due east of main entrance, See attached map)

8:00	8:15	Welcome and introductions (Guthrie and Dixon)
8:15	8:30	Welcome and remarks by Dr. Dae Chung (EM-2)
8:30	8:45	Welcome and remarks by Earren Mollot (FE-22)
8:45	9:30	NRAP overview presentation (George Guthrie)
9:30	10:15	ASCEM overview presentation (Paul Dixon)
10:15	10:45	Break
10:45	11:45	Breakouts: Description of current efforts of each program with respect to the breakout topic - led by breakout leads. These overviews will be sent out prior to workshop to all participants. (Conf rooms A410, E301 and E401)
11:45	1:00	Lunch
1:00	3:00	Breakouts: Discussion of similarities and differences in approach of the two programs with respect to the breakout topic. Areas of significant overlap identified. (Conf rooms A410, E301 and E401)
3:00	3:30	Break
3:30	4:30	Reconvene in conf room A410 Breakout leads report back to entire group - 20 minutes each with discussion.
4:30	5:00	Closing day comments and day 2 charge
5:00	6:00	Leadership team meeting - stock take and Day 2 planning.

September 2nd, 2010 (Conference room A410)

8:00	8:20	Instructions for Day 2 (Guthrie and Dixon)
8:30	11:30	Breakouts: Discussion of recommended collaborative initiatives to increase synergy and promote efficiency. (Conf rooms A410, E301 and E401)
11:30	1:00	Lunch
1:00	2:30	Reconvene in conf room A410 Breakout leads report back to the entire group. Summary of results and path forward recommendations - 30 minutes each with discussion.
2:30	3:00	Workshop summary (Guthrie and Dixon)
3:00	5:00	Leadership team meeting - compile results and set writing assignments for final report.

11. Appendix B: ASCEM/NRAP Workshop Charter

ASCEM/NRAP Program Integration Workshop

Overview

At the highest level, DOE-EM's Advanced Simulation Capability for Environmental Management (ASCEM) program and DOE-FE's National Risk Assessment Program (NRAP) for carbon dioxide (CO_2) sequestration have similar missions: to enable science-based risk assessment methodologies using best-in-class computational methods to integrate theory, experiments, and observations. This approach will focus research and development efforts by improving computational models, quantifying uncertainties and uncovering the most important knowledge gaps. The use of higher fidelity, science-based models will build confidence in risk assessments, as long as the models themselves are developed through a robust, iterative process to confirm the model's validity for its intended use. In both programs, systems-level models composed of submodels of individual components are required to link source terms, engineered and natural components, and receptors. Ideally, a flexible, computational platform linking multiphysics simulation software with modern uncertainty quantification and decision support tools will be adopted compatible with computer architectures from the desktop to the HPC scale. Finally, for reasons of cost, efficiency, reliability, and credibility, each program has adopted a "common architecture at many sites" paradigm in which standardization of software, methods, and approaches is promoted by developing a community software infrastructure that can be applied to multiple sites.

Workshop

Given the similarities in high-level goals of the two programs, there is a need to examine the commonalities and differences that emerge when these goals are applied in two distinct application areas: groundwater and soil remediation and CO_2 sequestration. A workshop with participation from the key science and program management leaders of both efforts is required to ensure integration across these two important national programs. Both programs are in their initial stages, and are expecting to ramp up considerably in the next few years, making this an opportune time for the workshop.

The workshop will consist of overview presentations from both efforts, followed by more detailed topical areas discussed in smaller breakout sessions. For each topic discussed, the following overarching questions will be answered:

- What is each program doing to address the challenges embodied in this topic?[1]

[1] High-level information will be compiled before the workshop from each of the two program plans, enabling workshop time to be devoted to more detailed discussions.

- What are the similarities and differences in the requirements of each program for this topic?
- What are the initiatives in each program that could be leveraged by the other to maximize efficiencies and promote common practices?

Below are descriptions for each of the three breakout sessions:

1) **Verification and Validation (V&V)/Model Confirmation**:

- What are the best approaches for building confidence in the applicability of these integrated, systems models?
- What is the appropriate mix of verification of algorithms versus comparison against data?
- Is confirmation of the individual subsystem models sufficient, or is a complete validation at the system level required?
- Who are the audiences for V&V activities, and are the needs of these audiences different?
- How can these modeling platforms be used to improve the integration of models with experiments and observations?

2) **Computational Platform**:

- What is the best approach for linking disparate subsystem models together into a system model?
- Are existing platforms sufficient, or is new code development essential?
- How important is it to exploit HPC resources, and what is the best way to do that?
- Is parallel computing required within an individual model run, or to execute multiple runs more quickly, or both?
- What new analyses (beyond Monte Carlo) will be enabled with a HPC platform?
- Are there drivers other than risk (i.e. cost, enablement of scientific discovery, transparency, usability, decision support?) that should be considered in the design of the platform? If so, how does that change the platform?
- How should the user interface with critical data (site characterization data, risk-related parameters, etc.) and how should the platform be designed to ensure the pedigree of the data inputs and model outputs?

12. Appendix C: ASCEM/NRAP Workshop Breakout Groups

ASCEM/NRAP Workshop Participation List			
Computational Platform (Conference Room A410)	**Breakout Lead**	**Skills Mapping**	**E-mail Addresses**
LANL – Rajesh Pawar,	x		rajesh@lanl.gov
PNNL - Ian Gorton (Platform Development Lead)	x		ian.gorton@pnl.gov
PNNL – Pete McGrail			pete.mcgrail@pnl.gov
LANL - Elizabeth Keating (Uncertainty Quantification Leads)			ekeating@lanl.gov
LBNL - Deb Agawal (Data Management Lead)			daagarwal@lbl.gov
LANL - Carl Gable (Model Development and Analysis Lead)			gable@lanl.gov
NETL – George Guthrie (NRAP Program Manger)			george.guthrie@netl.doe.gov
PNNL- Mark Rockhold			Mark.Rockhold@pnl.gov
LANL - Paul Dixon (ASCEM Multi-Lab Program Manager)			p_dixon@lanl.gov
PNNL - Tom Brouns (Manager of the Clean Fossil Energy Sector)			tom.brouns@pnl.gov
SRNL - Mary Harris (Director of Comp Sciences and CIO)			mary.harris@srnl.doe.gov
DOE EM - Mark Williamson (ASCEM Program Manager EM-32)			mark.williamson@em.doe.gov
DOE SC - David Lesmes (BER)			david.lesmes@science.doe.gov
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Multi-Physics Simulator and HPC Framework (Conference room 301)	**Breakout Lead**	**Skills Mapping**	**E-mail Addresses**
LBNL – Jens Birkholzer	x		jtbirkholzer@lbl.gov
LANL - David Moulton (HPC Development Lead)	x		moulton@lanl.gov
LLNL - Josh White (Geomechanical Modeling)			jawhite@llnl.gov
LBNL - Juan Meza (ASCEM Technical Integration Manager)			jcmeza@lbl.gov
DOE SC - Randall Laviolette (ASCR)			Randall.Laviolette@science.doe.gov
NETL -- Madhava Syamlal (HPC)			madhava.syamlal@netl.doe.gov
LANL - Andy Wolfsberg (ASCEM Lab Lead)			awolf@lanl.gov
ANL - Monica Regalbuto (EM-31 CBP Lead)			Monica.Regalbuto@em.doe.gov
			_
V&V / Model Confirmation (Conference Room E401)	**Breakout Lead**	**Skills Mapping**	**E-mail Addresses**
LLNL – Susan Carroll	x		carroll6@llnl.gov
LANL - Bruce Robinson (Deputy Division Director EES)	x		robinson@lanl.gov
NETL – Brian Strazisar (Wellbore Integrity)			Brian.Strazisar@netl.doe.gov
PNNL – Chris Brown (Groundwater Systems)			Christopher.brown@pnl.gov
PNNL - Mark Freshley (Site Applications Lead)			mark.freshley@pnl.gov
LBNL - Don DePaolo (Lab Director Earth Sciences)			djdepaolo@lbl.gov
DOE EM - Kurt Gerdes (Acting Office Director EM-32)			kurt.gerdes@em.doe.gov
DOE SC - Nick Woodward (BES)			nick.woodward@science.doe.gov
LANL-Bruce Letellier (uncertainty quantification)			bcl@lanl.gov
LANL-Scott Painter (modeling)			spainter@lanl.gov
LLNL-Yunwei, Sun (uncertainty quantification)			sun4@llnl.gov
DOE-FE - Ehsan Khan			ehsan.khan@hq.doe.gov

13. Appendix D: ASCEM/NRAP Workshop Breakout Group Reports

V&V/Model Confirmation Breakout Group

- *What is each program doing to address the challenges embodied in V&V/model confirmation?*
  - ASCEM: site applications effort will use field demonstration site data
  - NRAP: sequestration program provides access to field injection data. Field and laboratory testing programs are being developed.

- *What are the similarities in the needs of each program with respect to V&V/model confirmation?*
  - Better understanding of upscaling and the scale issues associated with heterogeneity, processes, and interpretation of measurements
  - Commonalities in the geochemical processes in shallow aquifers
  - Both systems require models that have an engineered component interacting with a natural system
  - UQ is critical to model confidence building

- *What are the differences in the needs of each program with respect to V&V/model confirmation?*
  - CO2 has more focus on pressure and geomechanical effects
  - EM problems are often focused on radionuclides

- *What are the initiatives in each program that could be exploited by the other to maximize efficiencies and promote common practices?*
  - Geochemical field data sets that might serve the needs of both programs in building model confidence – EPRI field site; Savannah River F Area. Cr contamination at LANL.
  - UQ methods in practice – test cases for incorporation of data from operating field sites. ASCEM – Sav. River field site. NRAP – EPRI site. Types of collaboration would include sharing of ideas, discussion of methods, perhaps with a workshop to ensure groups are learning from one another.
  - Topics: desired level of complexity, conceptual model uncertainty; uncertainty of geological structure
  - Model reduction: models of reduced order that capture the “essence” of the original process model and the data on which it is based
  - Upscaling methods and algorithm development of ASCEM will help NRAP – are there intermediate-scale tests planned that could be beneficially used by both programs?

- *What are the initiatives in each program that could be exploited by the other to maximize efficiencies and promote common practices (continued)?*

  - Decision support: programs should trade ideas for best methods and practices. Examples: optimization of monitoring, field management.
  - Cement: is there an opportunity to learn from each other. Are analogs a possibility?

Computational Platform Breakout Group

- *Discussions within breakout group involved topics associated with general topics such as:*
  - Terminology, general approaches, near & long term goals for developing tools/approaches
  - Specific issues such as data management approaches; coupled/uncoupled models; data integration from characterization/scientific efforts (living models); UQ including multiple conceptual models, correlated parameters; model complexities and verification of results (whether we are there yet?); overlap in terms of specific processes and flexibility to incorporate processes

- *What is each program doing to address the challenges embodied in computational platform?*
  - NRAP is utilizing existing modeling/simulation tools and platforms e.g GoldSim or manual integration of models for subsystems
  - ASCEM is developing a new computational platform that enables use of ASCEM HPC simulator, advanced data management, Wiki based collaborations, range of tool sets

- *What are the similarities in the needs of each program with respect to computational platform?*
  - Approaches to integrate separate models (different physics, including coupled processes) for multiple sub-components governed by different physics
  - Risk assessment/decision support framework e.g. optimization of monitoring wells for CO2 or pump & treat wells for EM
  - UQ
  - Data/knowledge integration approaches as new understanding/models are generated
  - Data management approaches, provenance

- *What are the differences in the needs of each program with respect to computational platform?*
  - Differences due to different data sources (characterization)
  - Different process models
  - Different risks
  - Different regulatory environments, stakeholders

- *What are the initiatives in each program that could be exploited by the other to maximize efficiencies and promote common practices?*

- Approaches for UQ, data management/integration, visualization, transparency

- *What are the initiatives in each program that could be exploited by the other to maximize efficiencies and promote common practices?*
  - Approaches for UQ
    - Conceptual model uncertainty
    - Treatment of correlated stochastic parameters
  - Approaches for model reduction/response surfaces
  - Data/knowledge management & integration
  - Visualization
  - Transparency & traceability
    - accessible tools/approaches to broader stakeholder base

- *What are the initiatives in each program that could be exploited by the other to maximize efficiencies and promote common practices?*

Initiatives	Priority	Timing
Approaches for UQ Sharing of lessons learned from ASCEM demo	1	1Q FY11
Approaches for model reduction/response surface Sharing of lessons learned from NRAP risk profile calculations	1	2Q FY11
Data/knowledge management & integration	2	1Q FY11
Visualization	3	FY12
Transparency & traceability • accessible tools/approaches to broader stakeholder base	4	FY12

Multi-Physics Simulator and HPC Framework Breakout Group

- *What is each program doing to address the challenges embodied in multi-physics HPC?*
  - ASCEM Core Mission: Will develop a new modular open-source community HPC simulator for various multi-physics processes running on computational platforms ranging from PCs to new Petascale Computers
  - NRAP Core Mission: Conduct necessary science to understand and quantify multi-physics processes relevant for developing a risk profile calculation methodology. NRAP is an integrated experimental (lab, field) and simulation approach, thereby mostly using existing simulators.
  - What are the similarities in the needs of each program with respect to multi-physics HPC?
  - Usefulness of HPC computations to enhance fidelity of solutions and enable UQ/optimization/sensitivity/inversion
  - Usefulness of community code with certain level of standardization and accountability across the complex
  - Need for multi-component transport, reactive geochemistry, thermodynamic databases, cementitious barriers
  - Need for handling coupled processes, weak and tight coupling approaches

- *What are the differences in the needs of each program with respect to multi-physics HPC?*
  - Level of coupling, priorities of multi-physics processes, different components, importance of multi-phase flow and phase changes
  - ASCEM: will implement various couplings between flow, reactive transport, thermal and mechanical processes, but the latter have lower priority
  - NRAP: stronger emphasis on geomechanical processes, important risk driver, will for certain system aspects require tight coupling
  - NRAP: stronger emphasis on true three-phase systems, stronger emphasis on phase changes, stronger emphasis on non-isothermal effects, larger range of pressure and temperature subsurface conditions, specific geochemistry related to presence of CO_2
  - What are the initiatives in each program that could be exploited by the other to maximize efficiencies and promote common practices?
  - ASCEM community code is modular enough to be expanded for some or all of NRAP's needs
  - ASCEM could benefit from NRAP's process understanding and modeling in some areas (geomechanics, higher P,T geochemistry, tight coupling)

- *What are the initiatives in each program that could be exploited by the other to maximize efficiencies and promote common practices? Where can synergies be exploited?*
  - Develop a strategy for communications/sharing of data, regular meetings of leaderships teams
  - Sharing of information on ASCEM requirements for HPC, NRAP requirements, ensuring that ASCEM decisions are not restrictive for later use

in NRAP (regular CO_2 community input, option is NRAP participation in ASCEM internal code review)
- Provide NRAP-CO_2 perspective (addition) to ASCEM process requirements document (lay out NRAP processes, coupling, feedback)
- Sequenced steps for closer integration, from communication/sharing to easy synthesis to additional scope for developing products
- For close integration, a roadmap needs to be developed with decision points, schedule, etc.
- Possible steps for close integration (start with low-hanging fruit, possibly addressing some, not all of NRAP's modeling needs):
- Identify CO_2 related problems that can be solved by ASCEM HPC without additions (e.g., reactive transport in GW after leakage of CO_2, elevated PCO_2, with sharing of thermodynamic database), provide NRAP test problems to V&V benchmarking document for ASCEM, ASCEM support to NRAP for use of HPC code, computational facility
- Add multi-phase capabilities to ASCEM (reservoir modeling), EOS, rel perm, etc., accelerate ASCEM schedule, provide NRAP benchmark problems (e.g., from code comparisons)
- Add non-isothermal
- Add geomechanics, starting with continuum elasticity